Data Dictionary: Physiological parameters for the human BDCM model

Parameter, units	Symbol	Value	Footnote
Height, cm	Height	160 - 190	[1]
Body Weight, kg	BW	65-91	[1]
Alveolar ventilation Rate, L/h-m^2	QPC	212.4	[2]
Alveolar Deadspace, unitless	Deadspace	0.238	
QPC to Cardiac Output Ratio, unitless	RQPCO	0.8	[3]
Fractional Blood Flows, unitless			[4, 5]
Richly Perfused Tissue Group	FQRP	0.75	[5,6]
Liver	FQL	0.09	
Gastrointestinal Tract	FQG	0.16	
Kidney	FQK	0.15	
Poorly Perfused Tissue Group	FQPP	0.25	[6]
Fat	FQF	0.05	
Blood Flow to Skin, L/min-m^2	QSKSA	0.58	[6]
Compartment Volume, unitless			[3]
Blood fraction of BW	FVBD	0.079	[7]
Blood as arterial	FVART	0.25	
Blood as venous	FVVEN	0.75	
Richly perfused fraction of BW	FVRP	0.20	[8]
Poorly perfused fraction of BW	FVPP	0.80	
GI tract fraction of BW	FVGI	0.0165	
Liver fraction of BW	FVL	0.026	
Fat fraction of BW	FVF	0.07 – 0.20	[1]
Kidney fraction of BW	FVK	0.004	
Volume GI tract lumen, L	VLUM	2.1	[3]
Skin thickness, mm	LSK	2.0	[9]

[1]Height and BW are experiment specific (Leavens et al. 2007). Average height and BW used for general simulations were 178 cm and 74 kg, respectively (based on the subject average) in Leavens et al. (2007). Individual subject-specific FVF data were also available from Leavens et al. (2007) estimated based on skin fold thickness. Average FVF used for general simulations was 0.11.

[2]Minute ventilation rate was scaled to skin surface area (SA) in m^2, $QP = QPC * SA * (1-Deadspace)$. SA was estimated on the basis of height and weight as $SA = 0.0239*(Height^{0.417})*(BW^{0.517})$ (USEPA, 2011).

[3]Cardiac Output, $QC = QP/RQPCO$.

[4]Physiological parameters from (Brown et al. 1997) unless otherwise specified.

[5]Fractional blood flows to individual tissues are scaled to cardiac output (QC), i.e. $QL = FQL *QC$, $QG= FQG *QC$, $QK= FQK * QC$, and $QF = FQF * QC$.

[6]Richly (QRP) and poorly perfused (QPP) tissues calculated respectively, as follows: $QRP = (FQRP*QC)-QL-QK-QG$ and $QPP = (FQPP*QC)-QF-QSK$. Blood flow to skin (QSK) is calculated as $QSK = QSKSA * SA * 60$ min/hr

[7]Volume of blood compartment is scaled to BW and volume of arterial (Vart) and venous (Vven) compartments are calculated respectively, as $VART = FVART*VBD$ and $VVEN = FVVEN*VBD$.

[8]Tissue volumes to tissues are scaled to BW with richly (VRP) and poorly perfused (VPP) tissue volumes calculated respectively, as follows: VRP = FVRP*BW-VL-VGI-VBD-VK and VPP = FVPP*BW-VF-VSK. Volume of skin (VSK) is calculated as VSK = LSK*SASK.

[9]LSK is average value for thickness of dermis and epidermis ([Laurent et al. 2007](#))

Data Dictionary: Chemical-specific parameters in the human BDCM model

Parameter, units	Symbol	Value			Footnote
		Male	Female	Average	
Partition coefficients, unitless					
Blood:Air	PBBDCM	17.33	14.61	15.97	[1]
Liver:Blood	PLBDCM	1.77	2.09	1.93	[2]
Gut:Blood	PGBDCM	1.77	2.09	1.93	[3]
Kidney:Blood	PKBDCM	1.90	2.25	2.08	[2]
Fat:Blood	PFBDCM	30.35	36.00	33.2	[2]
Skin:Blood	PSKBDCM	2.68	3.18	2.91	[4]
RPTG:Blood	PRPBDCM	1.77	2.09	1.93	[3]
PPTG:Blood	PPPBDCM	0.72	0.85	0.78	[2]
Skin diffusion coefficient, cm/h	KBDCM	0.18			[5]
Skin:water partition coefficient	PWSBDCM	5.6			[5]
Oral absorption coefficient, h^{-1}	KABDCM	8.3			[6]
Vmax CYP Liver, µg/h-kg $BW^{0.75}$	V1CBDCM	4.13×10^{4}			[1]
KM CYP Liver, µg/L	KM1BDCM	221			[1]
Kf GST Liver, 1/h-kg $BW^{0.75}$	VFCBDCM	0.0079			[7]

[1]Experimentally determined in this laboratory. See Methods for details.

[2]Calculated by dividing rat tissue:air partition coefficient (Lilly et al. 1997a) by human blood:air partition coefficient.

[3] Gut:air and rapidly perfused tissue:air partition coefficients were assumed to be the same as liver:air.

[4] Skin:air partition coefficient (Haddad et al. 2006) used with human blood air partition coefficient to calculate skin:blood partition coefficient.

[5] Skin diffusion coefficient determined with method using aqueous solution across human skin (Xu et al. 2002). Skin:water partition coefficient calculated on basis of water:air partition coefficient (Batterman et al. 2002) divided by skin:air partition coefficient (Haddad et al. 2006).

[6]Estimated on basis of Tmax from oral time course data of Leavens et al. (2007). See text for details.

[7]Estimated from in vitro clearance of BDCM from pooled human liver cytosol (Ross and Pegram 2003).